

**METHODS FOR A SYSTEMATIC, COMPREHENSIVE SEARCH  
FOR FAST, HEAVY SCINTILLATOR MATERIALS\***

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**ABSTRACT**

Over the years a number of scintillator materials have been developed for a wide variety of nuclear detection applications in industry, high energy physics, and medical instrumentation. To expand the list of useful scintillators, we are pursuing the following systematic, comprehensive search: (1) select materials with good gamma-ray interaction properties from the 200,000 data set NIST crystal diffraction file, (2) synthesize samples (doped and undoped) in powdered or single crystal form, (3) test the samples using sub-nanosecond pulsed x-rays to measure important scintillation properties such as rise times, decay times, emission wavelengths, and light output, (4) prepare large, high quality crystals of the most promising candidates, and (5) test the crystals as gamma-ray detectors in representative configurations. An important parallel effort is the computation of electronic energy levels of activators and the band structure of intrinsic and host crystals to aid in the materials selection process.

**DESIRED SCINTILLATOR PROPERTIES**

Scintillator materials are widely used for the detection of ionizing radiation in a variety of applications including high energy physics, astrophysics, geophysical exploration, medical imaging, security inspection, and industry. As different applications place very different priorities on density, atomic number, light output, decay time, emission wavelength, mechanical and chemical stability, radiation hardness, optical quality, and cost, it is unlikely that a single material will be found that is ideal for all applications. In this paper we shall be interested mainly in scintillator materials for detecting 511 keV gamma rays in positron emission tomography. Here stopping power and light yield are of prime importance. This is in contrast, for example, to materials needed for electromagnetic calorimetry in high energy physics experiments where light yield is of lesser importance but radiation hardness is a prime consideration.

High Stopping Power

For the detection of gamma rays with good spatial resolution, it is necessary to have a material with both a high density and an element with a high atomic number. Photoelectric absorption of the incident gamma is strongly preferred because the photon energy is deposited at a single position whereas Compton

interactions lead to several spatially separated energy depositions. Figure 1 illustrates how the photofraction  $\alpha = \mu_p / (\mu_p + \mu_c)$  for 511 keV photons depends on atomic number ( $\mu_p$  and  $\mu_c$  are the cross sections for photoelectric absorption and Compton scattering). The photoelectric attenuation length  $P$  is defined as the attenuation length/photoelectric fraction in cm for 511 keV photons. The probability of photoelectric absorption of 511 keV photons on the first interaction is

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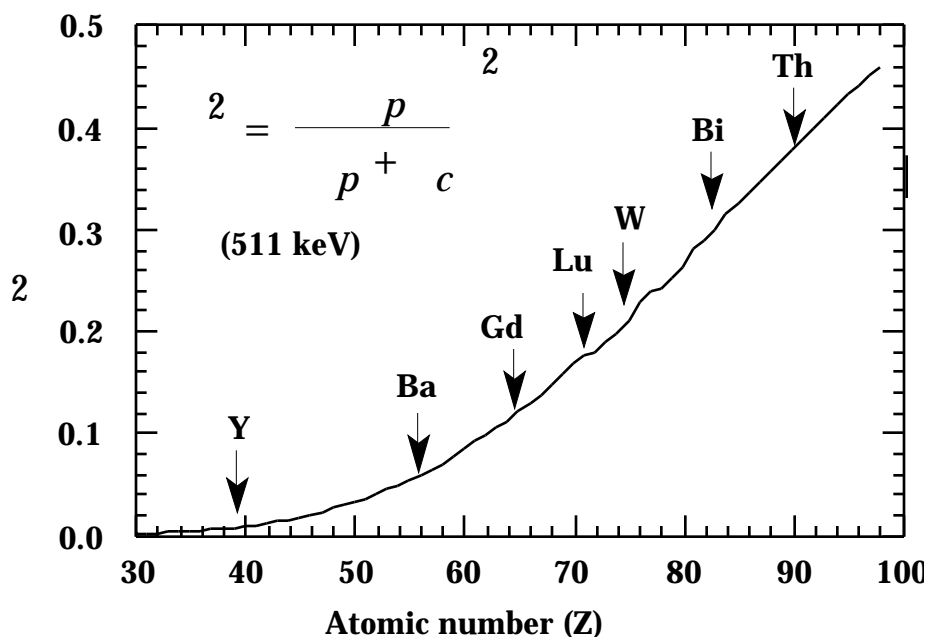


Figure 1. Photoelectric fraction for 511 keV photons as a function of atomic number.

only 23% for barium and iodine but 54% for lead and bismuth. It is thus clear why  $\text{Bi}_4\text{Ge}_3\text{O}_{12}$  (BGO) is favored for the detection and localization of higher energy gamma rays, especially for positron emission tomography where the coincident detection efficiency depends on  $\alpha^2$ . Note that there is surprisingly little improvement in efficiency to be gained by using thorium or uranium which, although being very heavy elements, are naturally radioactive and produce approximately  $10^6$  disintegrations per second per mole.

### Good Energy Resolution

Good energy resolution depends primarily on a high light output, given later in tables as  $L$  (photons per MeV). Another consideration is the detectivity of the scintillation light by matching the wavelength of emission with the spectral sensitivity of the photodetector. A bi-alkali cathode photomultiplier tube has a

quantum efficiency between 15% and 25% for wavelengths between 300 and 450 nm (the lower limit can be reduced to 200 nm by using a quartz faceplate). The standard silicon photodetector has a quantum efficiency between 60% and 80% for wavelengths between 400 and 700 nm, although enhanced response in the ultraviolet can be obtained by using special window coatings.

### Good Timing Resolution

Good timing resolution depends on the initial light intensity which is given later in Tables 1 and 2 as  $L(0.1)$ , the number of photons emitted in the first 0.1 ns. This factor is enhanced for materials with a large light output and a short decay time, that is, materials with a large radiative decay probability and high radiative quantum efficiency.

### Short Dead Time

For detecting gamma rays at high rates, it is important that the scintillation light is emitted quickly and with no long ( $\mu$ s, ms) afterglow. The quantities  $t(50\%)$  and  $t(90\%)$  in the tables are the times required for 50% and 90%, respectively, of the light to be emitted. The first time is relevant to measurements of energy; the latter is relevant to pulse pair resolution (avoiding pileup).

### Stability

Stability includes mechanical ruggedness, chemical inertness under normal atmospheric conditions, and radiation hardness. Mechanical and chemical stability are important when small crystals that can not be easily sealed individually are required. For instance, NaI(Tl) requires encapsulation, but this is not a problem when the material is used in the form of large crystals.

### Availability

For a scintillator to become available in large commercial quantities, it must be reasonably inexpensive to (i) purchase the starting compounds, (ii) grow large, clear crystals, and (iii) cut and polish them to form the desired geometry. Typically, the experience gained from the growth of many hundreds or thousands of crystals is necessary before the production of materials with the required size, lack of impurities and imperfections, and overall quality is achieved.

## **KNOWN SCINTILLATORS**

Table 1 lists properties of ten commonly used, heavy, commercially available scintillator materials.  $\text{BaF}_2$  is valued for its fast decay component which produces about 250 photons per MeV

Table 1. Operational characteristics of commercially available heavy scintillators.

Formula	D	P	L	L(0.1)	t(50%)	t(90%)
BaF <sub>2</sub>	4.89	11.8	12,000	250	320	1,340
Bi <sub>4</sub> Ge <sub>3</sub> O <sub>12</sub> (BGO)	7.13	2.6	8,200	3.7	184	664
CaWO <sub>4</sub>	6.1	4.7	6,000	0.1	4,160	13,800
CeF <sub>3</sub>	6.16	9.1	4,400	22	17	61
CsF	4.11	13	2,500	85	2.0	6.7
CsI(pure)	4.51	11	2,300	14	11	37
CsI(Tl)	4.51	11	64,800	7.5	616	2,400
Gd <sub>2</sub> SiO <sub>5</sub> (GSO)	6.71	5.8	10,000	117	42	138
NaI (77 K)	3.67	17	76,000	1,125	42	138
NaI(Tl)	3.67	17	38,000	17	159	530

D = density in g/cm<sup>3</sup>

P = attenuation length/photoelectric fraction in cm for 511 keV photons

L = luminosity in photons per MeV (emissions > 10  $\mu$ s excluded)

L(0.1) = luminosity in photons per MeV emitted in the first 0.1 ns

t(50%), t(90%) = time in ns for emission of 50%, 90% of the light, respectively

in the first 0.1 ns. BGO and CaWO<sub>4</sub> are valued for their stopping power, and CsI(Tl) and NaI(Tl) are valued for their high luminosities L. For a more detailed review of the properties of the materials in Table 1 and references to the literature, see reference [1].

Table 2 lists the properties of eight heavy scintillators that have been investigated but are not yet commercially available. Of these, only Lu<sub>2</sub>SiO<sub>5</sub>(Ce) (LSO) and PbWO<sub>4</sub> (PWO) have been grown in large, clear crystals. LSO is one of the most luminous cerium-activated compounds and may forever remain expensive due to its large lutetium content. It is, however, an important example that may lead to other highly luminous cerium-activated scintillators. ZnO(Ga) has been included because it has the largest initial intensity L(0.1) and among the shortest deadtime [t(90%)] of all known inorganic scintillators. Its initial intensity exceeds that of all core-valence transition scintillators by a large factor. For many applications, a scintillator with the stopping power of BGO and the fluorescence properties of ZnO(Ga) would be ideal. However, ZnO(Ga) is only available in polycrystalline (i.e., powdered) form.

Table 2. Operational characteristics of heavy scintillators not commercially available.

Formula	D	P	L	L(0.1)	t(50%)	t(90%)
BaCl <sub>2</sub>	3.90	17.4	14,000	700	2.0	800.
CeCl <sub>3</sub>	3.90	17.7	23,000	130	1	60
CuI	5.62	13	570	300	0.09	1.9
Lu <sub>2</sub> SiO <sub>5</sub> (Ce)	7.4	3.6	30,000	75	28	92
PbSO <sub>4</sub>	6.4	2.96	5,000	25	38	380
PbSO <sub>4</sub> (170 K)	6.4	2.96	68,000	12	513	2700
PbWO <sub>4</sub>	8.2	2.1	420	10	4.8	40
Yb <sub>2</sub> O <sub>3</sub>	9.2	2.6	100	50	0.09	0.4
ZnO(Ga)	5.6	87	15,000	2,400	0.4	1.5

Column headings are the same as defined in Table 1.

## A COMPREHENSIVE, SYSTEMATIC SEARCH APPROACH

Figure 2 illustrates our search strategy for discovering and characterizing new scintillator materials. It begins by using the NIST crystal diffraction file as a list of possible compounds. A selection of materials or groups of materials is then made based on (1) their physical properties, (2) prior knowledge of their luminescence characteristics, (3) experimental measurements, and (4) theoretical calculations.

### The NIST Crystal Diffraction Database

The NIST crystal diffraction database is available on a CD-ROM and contains 200,000 data sets describing over 50,000 distinct compounds[2]. It serves as a list of compounds that exist, i.e., they have been synthesized in crystalline form and analyzed by their x-ray diffraction pattern. Compound formulas, crystallographic space group and cell parameters, density, and references may be extracted from the database.

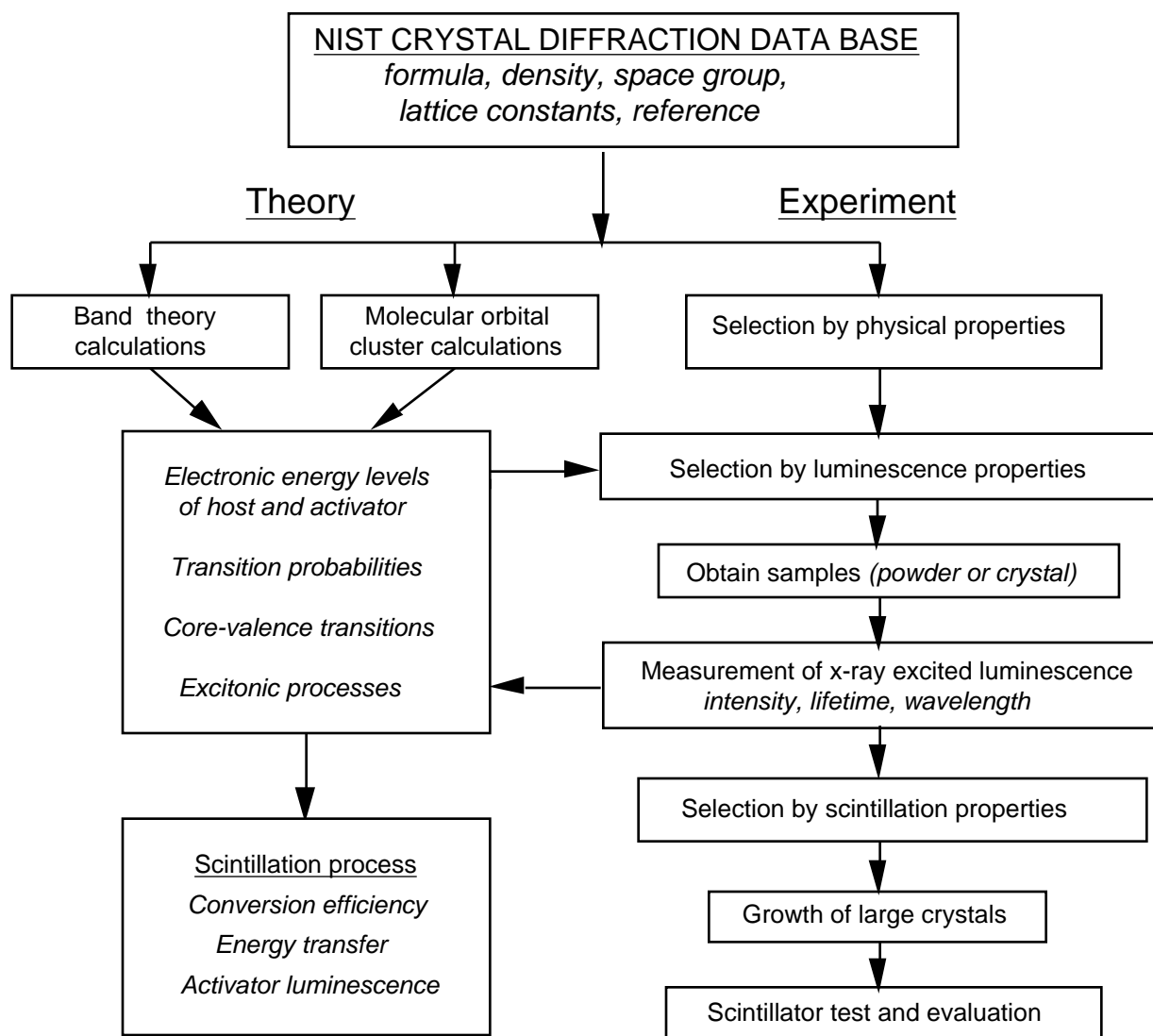


Figure 2. Schematic of scintillator material search strategy.

### Selection by Physical Properties

Materials from the NIST crystal diffraction database are selected and sorted based on their composition and various physical properties and parameters. A program was written to transfer the information in the database to a commercial database program for filing and sorting. Individual materials can be called up by chemical name or formula. Groups of materials can be called up by general type (e.g., oxides or fluorides), by elemental composition (e.g., materials containing Bi and Al, elements of interest for core-valence transitions, etc.), or by property (e.g., materials of density greater than  $8 \text{ g/cm}^3$ , materials having a photoelectron attenuation length less than 5 cm, etc.). Furthermore, materials can be eliminated from a grouping because of undesirable properties (e.g., absorptive transition metals or radioactive elements). Materials in the resultant groupings can then be sorted by increasing or decreasing values of some property or characteristic.

An immense, diverse literature of the luminescence properties of various inorganic and organic materials has been generated over the past half century. This has resulted in a very large number of known luminescent ions and molecular groups having emissions covering a wide wavelength range. While these investigations have usually been of photoluminescence rather than radioluminescence, this information provides a pre-screening of those luminescent ions having emission wavelengths, decay times, and radiative efficiencies in the range of possible interest. The general behavior of these properties with variations in the host material are frequently known phenomenologically. This latter knowledge is also used to guide our selection of candidate compounds, but for new materials actual measurements are still required.

As evident from Fig. 1, hosts containing bismuth and lead are attractive for stopping 511 keV gamma rays. In Table 3 we list a number of lead and bismuth compounds derived from the database that have high density  $D$  and small photoelectric attenuation lengths  $P$ . These are just a few compounds that, based on these properties, are excellent candidates for our application but which in most cases have not been investigated for x-ray excited fluorescence intensity. These materials, even if they are not efficient intrinsic scintillators, may be attractive hosts for activators such as cerium.

As can be seen from Table 3, for a given group of ions, several compositional combinations may be possible. For example, of the  $\text{Bi}_2\text{O}_3\text{--GeO}_2$  compositions, the 6:1 compound has the greatest density but the 2:3 compound has the greatest luminous intensity at room temperature. Luminescence properties vary with the local structure at the activator site. In bismuth and lead compounds, the most efficient luminescence at room temperature is obtained from hosts in which the  $\text{Bi}^{3+}$  or  $\text{Pb}^{2+}$  sites have a very asymmetric arrangement of neighboring ions in the ground state[3]. Thus another selection can be made based of the local structure. We derive the local structure at a particular ion site from another program [4] which, given the space group, unit cell parameters, and positions of ions in inequivalent lattice sites, calculates the bond distances and angles for all ions within a chosen radius about the desired ion. This information also provides input to programs for electronic structure calculations discussed below. By assigning point charges appropriate to the ions, a principal axes transformation can be applied to the charge distribution; the resulting eigenvalues provide a measure of the asymmetry at the activator site[5].

### Sample Preparation

The difficulty of growing large, high-quality crystals is well recognized. While it is significantly easier to prepare the same compound in powder or polycrystalline form, it still could take a skilled chemist several days to prepare one compound and verify its identity. We view the limited availability of sample compounds as the primary limitation in the experimental search for new scintillators. Possibly the richest source of uncommon, heavy compounds might be found in existing collections of materials synthesized over the years for other purposes or applications.

Table 3. Selected compounds from the NIST crystal diffraction database.

Lead Compounds			Bismuth Compounds		
Material	P (cm)	D(g/cm <sup>3</sup> )	Material	P (cm)	D (g/cm <sup>3</sup> )
PbF <sub>2</sub>	1.8	8.5	BiF <sub>3</sub>	1.9	8.3
Pb <sub>2</sub> OF <sub>2</sub> (1:1)	1.8	8.2	BiOF (1:1)	1.6	9.2
Pb <sub>3</sub> BiO <sub>3</sub> F <sub>3</sub> (1:1)	1.5	9.6	BiPbFO <sub>2</sub> (1:1:1)	1.5	9.4
Pb <sub>5</sub> Bi <sub>8</sub> O <sub>17</sub> (5:4)	1.3	10.5	Bi <sub>6</sub> Pb <sub>2</sub> O <sub>11</sub> (3:2)	1.5	9.1
Pb <sub>5</sub> GeO <sub>7</sub> (5:1)	1.7	8.8	Bi <sub>12</sub> GeO <sub>20</sub> (6:1)	1.5	9.2
Pb <sub>11</sub> Ge <sub>3</sub> O <sub>17</sub> (11:3)	1.8	8.6	Bi <sub>2</sub> GeO <sub>5</sub> (1:1)	2.0	8.2
Pb <sub>5</sub> Ge <sub>3</sub> O <sub>11</sub> (5:3)	2.4	7.4	Bi <sub>4</sub> Ge <sub>3</sub> O <sub>12</sub> (2:3)	2.5	7.2
PbGeO <sub>3</sub> (1:1)	3.0	6.8	Bi <sub>2</sub> Ge <sub>3</sub> O <sub>9</sub> (1:3)	3.6	6.4
Pb <sub>3</sub> SiO <sub>5</sub> (3:1)	1.9	8.1	Bi <sub>2</sub> O <sub>3</sub>	1.5	9.2
Pb <sub>2</sub> SiO <sub>4</sub> (2:1)	2.1	7.6			
Pb <sub>3</sub> Si <sub>2</sub> O <sub>7</sub> (3:2)	2.4	6.7	Bi <sub>3</sub> YO <sub>6</sub> (3:1)	2.0	8.1
PbSiO <sub>3</sub> (1:1)	2.8	6.3	Bi <sub>3</sub> LuO <sub>6</sub> (3:1)	1.7	9.1
Pb <sub>8</sub> P <sub>2</sub> O <sub>13</sub> (8:1)	1.8	8.3	Bi <sub>5</sub> PO <sub>10</sub> (5:1)	1.6	9.2
Pb <sub>4</sub> P <sub>2</sub> O <sub>9</sub> (4:1)	2.2	7.3	BiPO <sub>4</sub> (1:1)	2.7	6.6
Pb <sub>5</sub> P <sub>4</sub> O <sub>15</sub> (5:2)	2.7	6.6			
			Bi <sub>24</sub> B <sub>2</sub> O <sub>39</sub> (12:1)	1.4	9.7
Pb <sub>6</sub> B <sub>10</sub> O <sub>21</sub> (6:5)	2.9	6.1	Bi <sub>4</sub> B <sub>2</sub> O <sub>9</sub> (2:1)	1.8	8.2
			Bi <sub>3</sub> B <sub>5</sub> O <sub>12</sub> (3:5)	2.8	6.2
Pb <sub>5</sub> SO <sub>8</sub> (5:1)	1.8	8.1			
Pb <sub>3</sub> SO <sub>6</sub> (3:1)	2.1	7.6	Bi <sub>2</sub> SO <sub>6</sub> (1:1)	2.1	7.7
Pb <sub>2</sub> SO <sub>5</sub> (2:1)	2.3	7.0	Bi <sub>2</sub> S <sub>2</sub> O <sub>9</sub> (1:2)	3.2	5.8
Pb <sub>3</sub> C <sub>2</sub> O <sub>7</sub> (3:2)	2.3	6.9	Bi <sub>2</sub> CO <sub>5</sub> (1:1)	1.8	8.2
PbCO <sub>3</sub> (1:1)	2.6	6.5			
			Bi <sub>2</sub> SiO <sub>5</sub> (1:1)	2.0	7.9
Pb <sub>5</sub> Ta <sub>4</sub> O <sub>15</sub> (5:2)	1.8	9.4			
Pb <sub>3</sub> Ta <sub>2</sub> O <sub>8</sub> (3:1)	1.9	9.0	BiTaO <sub>4</sub> (1:1)	1.9	9.1
PbTa <sub>2</sub> O <sub>6</sub> (1:1)	2.1	9.0			
			Bi <sub>24</sub> Al <sub>2</sub> O <sub>39</sub> (12:1)	1.5	9.7
Pb <sub>2</sub> TaAlO <sub>6</sub> (4:1:1)	2.2	9.2	BiAlO <sub>3</sub> (1:1)	2.1	8.1
Pb <sub>2</sub> TaLuO <sub>6</sub> (4:1:1)	1.7	10.1	Bi <sub>2</sub> Al <sub>4</sub> O <sub>9</sub> (1:2)	3.2	6.4
Pb <sub>6</sub> La <sub>2</sub> O <sub>9</sub> (6:1)	1.9	8.7	Bi <sub>2</sub> CdO <sub>4</sub> (1:1)	1.6	10.2
PbHfO <sub>3</sub> (1:1)	1.8	9.7	Bi <sub>12</sub> BaO <sub>19</sub> (6:1)	1.4	10.5
PbWO <sub>4</sub>	2.1	8.4	Bi <sub>2</sub> WO <sub>4</sub>	1.7	9.3



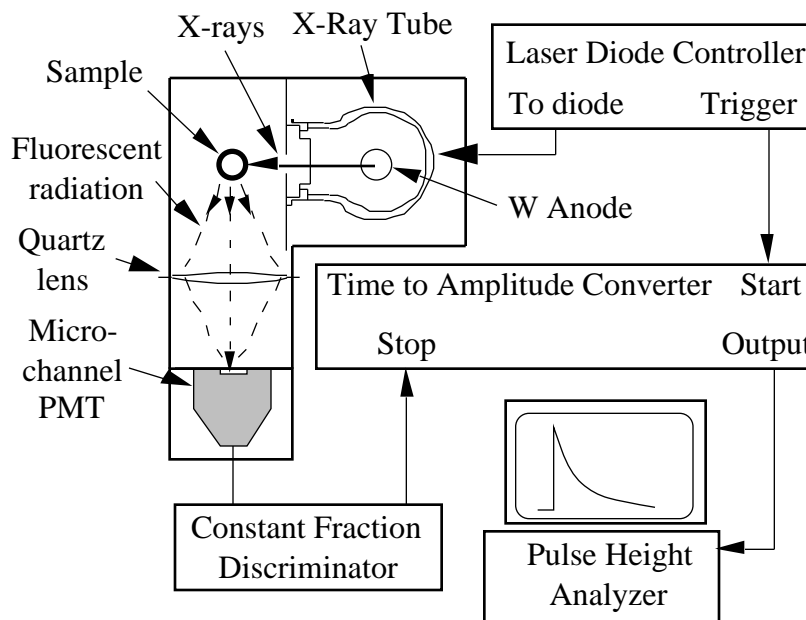


Figure 3. Pulsed x-ray apparatus (ref. 8).

### Sample Measurement

For several years we used synchrotron light sources (the Stanford Synchrotron Research Laboratory and the Brookhaven National Synchrotron Light Source) to provide pulses of x-rays for measuring the fluorescence characteristics of over 400 samples [6,7]. More recently we have developed an in-house laboratory apparatus shown in Fig. 3 and described in detail in ref. [8]. Light from a pulsed laser diode incident on a photoemissive surface generates a  $\sim 100$ -ps pulse of electrons that are accelerated and strike a tungsten anode, thereby producing a 30-keV x-ray pulse. For intensity measurements a cw or high-repetition-rate light source can be used to increase the excitation intensity (limited by the current capability of the x-ray tube). Up to 64 samples can be mounted in a computer-controlled carousel sample changer and automatically sequenced and measured. The emission is observed with a photomultiplier tube as shown. Various optical filters or a monochromator can be inserted into the optical path to determine the spectral region of the emission. Provisions also exist for making measurements with the sample at low or elevated temperatures.

### Growth and Testing of Large Crystals

Growing quality crystals is one of the major challenges in the development of new, improved scintillators. Our approach has been to seek and test compounds initially in any available form (powder, polycrystalline, or single crystal) and to leave the development of optimum crystal growth techniques for selected materials to the specialists. Once a crystal larger than roughly 5 mm is available, it can be covered by a reflector, coupled to a phototube, and its response to gamma radiation measured relative to well characterized and established materials. This includes

luminosity, energy resolution, timing resolution, fluorescence decay times, and absorption and emission wavelengths. To be a useful material, the existence and width of a well defined photopeak are essential additional criteria.

### Determination of Scintillation Mechanisms

The determination of scintillation mechanisms is important in understanding the limits to performance of a particular material and in guiding the development of a theory capable of predicting the properties of other compounds. Experimental measurements include the optical absorption spectrum which locates the excited states of the activator and/or absorption edge of the host material, the photoluminescence and radioluminescence spectra, and the photoluminescence and radioluminescence decay kinetics. As shown in ref. 9 and in other papers in this volume, excitation spectra recorded from the visible through the soft x-ray region provide valuable information for understanding the scintillation mechanism and overall quantum efficiency. The latter measurements are best performed using crystals in a vacuum ultraviolet beam of an electron synchrotron. These measurements plus others such as thermoluminescence and overall scintillation efficiency can be used to derive the efficiency of energy transfer to the luminescent species.

### **THEORETICAL CALCULATIONS**

Theoretical calculations of electronic energy levels of the activator and host can contribute to understanding the scintillation mechanism and efficiency. Various defects that can affect radioluminescence efficiency and susceptibility to radiation damage are also amenable to theoretical calculations. Although the values obtained with existing computer codes may not yet be of high accuracy, they can provide useful guidance in the search for improved materials.

For the activator ion, quantum-mechanical molecular-orbital cluster calculations using either ab initio or semi-empirical approaches have been applied. These approaches to treating transition metal and lanthanide ions are discussed by Bartram [10], Andriessen, et al., [11] and others elsewhere in these proceedings. In applying cluster models, there are questions of the number of ions in the cluster necessary to adequately describe the local environment, the embedding of the cluster in the host, and the location of the activator energy levels with respect to those of the host. For substitutional impurities, lattice relaxation of both ground and excited states must be treated.

Cluster calculations are also useful when investigating materials in which core-valence luminescence may occur. Both energy levels and radiative probabilities associated with core-valence transitions have been calculated with encouraging success[12].

If the material has translational symmetry, as in the case of intrinsic materials (e.g., CeF<sub>3</sub>, BGO, core-valence luminescence crystals), band theory can be used to

calculate the electronic energy levels and density of states. The fundamental band gap of a potential host material and possible core-valence transitions can also be predicted. To treat materials in which a dilute substitutional impurity has been added as an activator, a number of unit cells can be considered in which one has the substituted activator ion; this supercell is then treated as a translational unit and band theory again applied. In this case and in cases where there are many ions in the fundamental unit cell, such calculations become lengthy.

Mishra [13] has given examples of the application of both cluster model and band theory calculations to shown the insights gained by the complementary use of the two approaches.

With increasing computing power and storage capacity and well validated computer codes, theoretical predictions of scintillation properties are becoming easier. Calculations done with simplified programs are particularly useful for rapidly identifying systematic changes of properties with compositional variations.

## CONCLUSIONS

Many heavy compounds exist but the scintillation properties of only a small fraction have ever been measured. There are doubtless many useful scintillators among these waiting to be discovered. Two major challenges for initial measurements of scintillation properties are (1) acquiring a large variety of both doped and undoped compounds, and then (2) growing clear crystals of those few compounds exhibiting attractive x-ray excited fluorescence properties. Compared with these challenges, the task of exposing samples to a pulsed x-ray beam and measuring their fluorescence properties is relatively quick and easy. While reliable and reasonably accurate theoretical predictions of electronic energy levels are becoming available for guidance, experiment will remain as the final arbiter in the selection and evaluation of useful scintillator materials for the foreseeable future. The combination of experimental measurements and theoretical calculations should, however, lead to an increased understanding of scintillation processes and selection rules for discovering improved materials.

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